Potential Scattering and the Kondo Effect

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We study a generalized Kondo model in which a spin-$\frac{1}{2}$ impurity is coupled to a conduction band by both s-d exchange and potential interactions. A strong potential scattering is shown to screen an exchange scattering, and the Kondo temperature of the system is decreased.

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It is well known that the behavior of a magnetic impurity in a metal can be described by an effective 1D Hamiltonian,

$$H=\sum_{\sigma}\int\frac{dk}{2\pi}kc^{\dagger}_{\sigma}(k)c_{\sigma}(k)+\frac{1}{2}I\sum_{\sigma,\sigma'}\int\frac{dk}{2\pi}\frac{dk'}{2\pi}c^{\dagger}_{\sigma}(k)\left(\vec{\sigma}_{\sigma\sigma'}\cdot\vec{S}\right)c_{\sigma'}(k')+V\sum_{\sigma}\int\frac{dk}{2\pi}\frac{d\epsilon'}{2\pi}c^{\dagger}_{\sigma}(k)c_{\sigma}(k'). \tag{1}$$

Here, $\vec{\sigma}$ are the Pauli matrices, $\vec{S}$ is the impurity spin operator, and I is the s-d exchange coupling constant. The operators $c^{\dagger}_{\sigma}(k)$ refer to conduction electrons with spin $\sigma=\uparrow,\downarrow$ in a s-wave state of momentum modulus k. The last term in Eq. (1) corresponds to a potential (spin independent) scattering of an electron on the impurity site, V being the coupling constant. The electron energies and momenta in Eq. (1) are taken relative to the Fermi values, which are set to be equal to zero, while the Fermi velocity $v_F=1$. For simplicity, we confine ourselves to the case of $S=1/2$ which is of the most physical interest.

In the absence of a potential coupling, $V=0$, the model (1) is solved exactly [1,2] by the Bethe ansatz (BA). In the BA approach to the theory of dilute magnetic alloys [3,4], the spectrum of a host is alternatively described in terms of charge and spin excitations rather than in terms of free particles with spin "up" and 'down". The BA equations for charge, k_j, $j=1,\dots,N$, and spin λ_α, $\alpha=1,\dots,M$, rapidities describing N particles on an interval of size L have the form [5]

$$\exp\left(ik_jL\right)\Phi_{\rm ch}=\left(\frac{\lambda_\alpha+\frac{i}{2}}{\lambda_\alpha-\frac{i}{2}}\right)^M \tag{2a}$$

$$\left(\frac{\lambda_\alpha+\frac{i}{2}}{\lambda_\alpha-\frac{i}{2}}\right)^N\Phi_{\rm sp}(\lambda_\alpha)=-\prod_{\beta=1}^{M}\frac{\lambda_\alpha-\lambda_\beta+i}{\lambda_\alpha-\lambda_\beta-i} \tag{2b}$$

where M is the number of particles with spin "down". The eigenenergy E and the z component of the total spin of the system S^z are found to be

$$E=\sum_{j=1}^{N}k_j,\quad S^z=\frac{1}{2}+\frac{N}{2}-M. \tag{2c}$$

In Eqs. (2) the phase factors

$$\Phi_{\rm ch}=\frac{1-\frac{i}{2}U_0}{1+\frac{i}{2}U_0}\simeq\exp\left(-iU_0\right) \tag{3a}$$

$$\Phi_{\rm sp}(\lambda)=\frac{\lambda+\frac{1}{\mathrm{g}_0}+\frac{i}{2}}{\lambda+\frac{1}{\mathrm{g}_0}-\frac{i}{2}} \tag{3b}$$

describe the scattering of charge and spin excitation of the host on the impurity. Here

$$U_0=\frac{1}{4}I,\quad \mathrm{g}_0=\frac{1}{2}I. \tag{3c}$$

In the absence of the exchange coupling, $I=0$ or $S=0$, multiparticle effects are also absent. The model (1) is diagonalized in terms of independent particles with spin "up" and "down" scattering on the impurity potential. Pure

potential impurities are clear to change physical properties of a host only if they significantly modify the density of band states near the Fermi level. Therefore, dramatic changes in the thermodynamics of a host under a doping with magnetic impurities is associated with an s-d exchange coupling only, while the potential scattering term is assumed can be omitted.

Here, we note that not changing the structure of the BA equations (2) a potential scattering renormalizes the parameters U_0 and g_0. In the presence of potential scattering these parameters are replaced, respectively, by

$$U = U_0 + V \tag{4a}$$

$$\mathrm{g} = \frac{\mathrm{g}_0}{1+\frac{1}{4}(V+\frac{1}{4}I)(V-\frac{3}{4}I)}. \tag{4b}$$

At $V=0$, Eqs. (4) reduce to expressions given in Eq. (3c), provided that, as it is assumed in deriving Eqs. (2), $I \ll 1$. In the domain $I \ll |V| \ll 1$, the impurity term in Eq. (2a) for charge excitation is determined by potential scattering, $U \simeq V$, while scattering of spin excitations at the impurity is still determined by exchange coupling, $\mathrm{g} \simeq \frac{1}{2}I$. Finally, at $|V| \gg 1$, the effective coupling constant is given by $\mathrm{g} = 2I/V^2 = 4\mathrm{g}_0/V^2$, and hence the exchange scattering is screened by the potential one.

Thus, a strong potential scattering does not affect the qualitative behavior of the system, but it renormalizes physical parameters of the Kondo effect. In particular, the Kondo temperature is now found to be

$$T_K \sim \epsilon_F \exp\left(-\frac{\pi}{\mathrm{g}}\right) = \epsilon_F \exp\left(-\frac{\pi V^2}{2\mathrm{I}}\right), \tag{5}$$

where ϵ_F is the Fermi energy, while in the absence of potential scattering $T_K^0 \sim \epsilon_F \exp\left(-2\pi/I\right)$.

To derive Eqs. (4), it is enough to study how a potential scattering is incorporated in the particle-impurity scattering matrix. Let us look for one-particle eigenstates of the system in the form

$$|\Psi_1\rangle = \sum_{\sigma}\sum_{s=0,1}\int \frac{dk}{2\pi}\psi_{\sigma;s}(k)c_\sigma^\dagger(k)\left(S^+\right)^s|0\rangle,$$

where the vacuum state $|0\rangle$ contains no electrons and the impurity spin is assumed to be "down". The Schrödinger equation is then easily found to be

$$(k-\omega)\psi(k) + \frac{1}{2}I\left(\vec{\sigma}\cdot\vec{S}\right)A + VA = 0 \tag{6a}$$

$$A = \int \frac{dk}{2\pi}\psi(k), \tag{6b}$$

where ω is the eigenenergy, and spin indexes are omitted.

Inserting the general solution of Eq. (6a),

$$\psi(k) = 2\pi\delta(k-\omega)\chi - \frac{V}{k-\omega-i0}A - \frac{\frac{1}{2}I}{k-\omega-i0}\left(\vec{\sigma}\cdot\vec{S}\right)A,$$

with an arbitrary spinor χ, into Eq. (6b), one obtains

$$\left\{1+\frac{i}{2}\left[V+\frac{1}{2}I\left(\vec{\sigma}\cdot\vec{S}\right)\right]\right\}A = \chi.$$

For the Fourier image of the function $\psi(k)$,

$$\psi(x) = \int_{-\infty}^{\infty}\frac{dk}{2\pi}\psi(k)\exp\left(ikx\right),$$

a solution of Eqs. (6) is then found to be

$$\psi(x) = e^{ikx}\left\{\begin{array}{r} \chi, \;\; x<0 \\ \mathbf{R}\chi, \;\; x>0 \end{array}\right.$$

where $k=\omega$. Here, the electron-impurity scattering matrix is given by

$$\mathbf{R} = u + 2v\left(\vec{\sigma}\cdot\vec{S}\right), \tag{7a}$$

where the parameters u and v are found from the equations

$$u + v = \frac{1 - \frac{i}{2}(V + \frac{1}{4}I)}{1 + \frac{i}{2}(V + \frac{1}{4}I)} \tag{7b}$$

$$u - 3v = \frac{1 - \frac{i}{2}(V - \frac{3}{4}I)}{1 + \frac{i}{2}(V - \frac{3}{4}I)}. \tag{7c}$$

Diagonalization of the system with the particle-impurity scattering matrix $\mathbf{R}$ results in the BA equations (2) with scattering parameters given in Eqs. (4).

A screening of the exchange scattering and a lowering the Kondo temperature by quite a strong potential scattering, $|V| \gg I$, find a natural physical explanation. In the absence of the potential scattering, multiparticle effects in a spin subsystem of a metal doped with a Kondo impurities are generated due to an essential difference of electron-impurity scattering amplitudes in the triplet, $u + v$, and singlet, $u - 3v$, channels of scattering. As V grows, this difference in scattering amplitudes is easily seen from Eqs. (7) to be decreased and become negligible small at $|V| \gg I$. Therefore, the impurity term $\Phi_{\rm sp}$ disappears from Eq. (2b) describing the behavior of the spin subsystem, and the impurity is decoupled from the band states.

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